Towards 2D Boron Chemistry: A Computational Approach

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Abstract: Boranes are chemical compounds made from the basic elements boron and hydrogen. From the 1950s onward, William Lipscomb *et al* studied their composition by means of X-rays techniques, mapping their structures and leading to the concept of many-electron multi-center bonding[1] (boron does not follow the octet rule). Due to its electronic configuration, boron combines with itself, hydrogen and other elements of the Periodic Table forming open concave and closed polyhedral structures with triangular faces. Thus, 3D molecular shapes are usual within the world of boron clusters chemistry – not to be confused with organoboron chemistry. Previous and recent experimental and computational findings, such as the isolation of borophane[2] or metal complexes with planar pentagonal and hexagonal borane ligands,[3,4] however, have shown that the development of a 2D boron chemistry is not an entelechy. Thus, a theoretical one-to-one mapping can be drawn between any open or polycyclic conjugated hydrocarbon molecule C_nH_m and the corresponding borane B_nH_{m+n} using the number of valence electrons in a confined space[5] or a Hückeloid model.[6] In the same way that graphene finite patterns exist such as benzene, naphthalene or coronene, we may ask if finite patterns from borophane could be isolated.[7] The problem is that the simplest unit of borophane is unknown cyclohexaborane(12).[8] The stability of isolated hexagonal planar rings may depend on substituents - *exo* terminal hydrogens or e.g. NH_2 groups – and the presence of bridge hydrogen atoms, as in known diborane(6) B_2H_6.[9] Also the partial boronation of nucleic acid bases may throw some light on the role of boron in chemical processes involving biomolecules.[10] We thus propose the use of quantum-chemical computations to characterise and predict the properties of unknown planar finite boranes, heteroboranes as well as boronation of planar molecules with biochemical relevance to help synthetic chemists in the development of a potential new 2D boron chemistry.

References

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